



Silicon Nanoparticles as Hyperpolarized Magnetic Resonance Imaging Agents

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Supporting Information: Hyperpolarized Long- T_1 Silicon Nanoparticles for Magnetic Resonance Imaging

J. W. Aptekar,^{1,*} M. C. Cassidy,^{1,*} A. C. Johnson,¹ R. A. Barton,¹ M. Y. Lee,¹
C. Vo,¹ M. N. Anahtar,² Y. Ren,² S. N. Bhatia,² C. Ramanathan,³ D. G. Cory,³
A. L. Hill,⁴ R. W. Mair,⁴ M. S. Rosen,^{1,4} R. L. Walsworth,^{1,4} and C. M. Marcus^{1,†}

¹*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

²*Harvard-MIT Division of Health Sciences and Technology,
Massachusetts Institute of Technology E19-502D Cambridge, MA 02139, USA*

³*Department of Nuclear Science and Engineering,
Massachusetts Institute of Technology, Cambridge, MA 02139, USA*

⁴*Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, MS 59, Cambridge, MA 02138, USA*
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S1. Electron Spin Resonance Measurements

Continuous wave electron spin resonance (cw-ESR) measurements were taken on bulk samples of particles using a JEOL **FE-3XG** X-Band spectrometer at a frequency of 9.106 GHz. The a.c. field (amplitude 0.01mT, $f_{mod} = 100$ kHz) was swept from 315 mT to 335 mT over a period of 30 s. For each sample, a single peak at $B = 324$ mT, corresponding to a g-factor of 2.006 was recorded. This is consistent with the reported g-factor of P_b defects at the silicon-silicon dioxide interface [1]. ESR spectra of ball milled silicon particles with sizes $0.17\ \mu\text{m}$ and $1.6\ \mu\text{m}$. are shown in Fig. S1. Curves are scaled vertically by sample weight, giving a measure of density of electron spins. Smaller particles have greater defect density, scaling roughly as the inverse diameter (inset, Fig. S1), suggesting that the defects are on the surface of the nanoparticle [2].

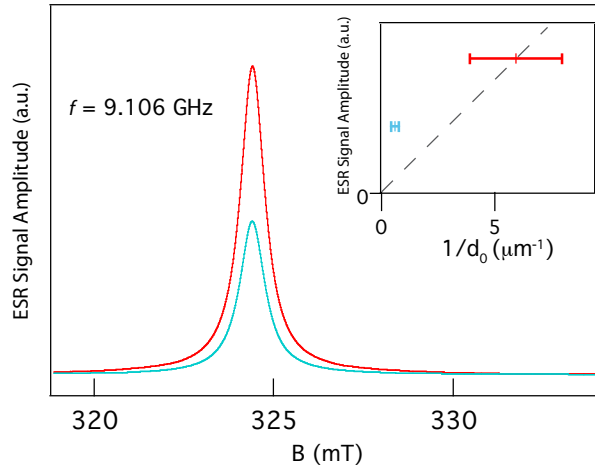


FIG. S1: **Electron spin resonance measurements of silicon particles.** Weight adjusted ESR spectra of ball milled silicon particles with sizes $0.17\ \mu\text{m}$ and $1.6\ \mu\text{m}$. Inset: ESR peak area vs inverse particle diameter.

S2. Evidence of Peylation via Stability of Particles

The aminated particles in this experiment were pegylated with either mPEG-SMB or NHS-PEG-MAL. Both SMB and NHS are reactive with amines on the particle surface. As a negative control, mPEG-Amine polymer was used because it does not contain amine-reactive groups and therefore should not conjugate to the nanoparticle surface. The stability of nanoparticles in solution was assessed using both dynamic light scattering (DLS) and visual determination of flocculation and sedimentation. The DLS-based size measurements of aminated and pegylated particles are shown in Table S1. As expected, the aminated particles treated with mPEG-Amine aggregated after centrifugation and

resuspension in phosphate-buffered saline (PBS). However, the particles treated with mPEG-SMB and NHS-PEG-MAL were both stable in PBS.

TABLE S1: DLS size measurements showing size before and after pegylation.

Silane	PEG ^a	Size after pegylation (nm)		
		Measured in MeOH	Measured in PBS	After two days in PBS
APTES only	None	220 ± 88	-	-
	Amine	Aggregated	Aggregated	Aggregated
	SMB	360 ± 127	271 ± 84	260 ± 70
	NPM	240 ± 95	396 ± 126	371 ± 140
APTES & BTEOSE	None	235 ± 100	-	-
	Amine	Aggregated	Aggregated	Aggregated
	SMB	300 ± 151	314 ± 165	520 ± 200
	NPM	255 ± 100	Aggregated	326 ± 117
APTES & THPMP	None	235 ± 100	-	-
	Amine	Aggregated	Aggregated	Aggregated
	SMB	490 ± 200	295 ± 200	360 ± 200
	NPM	295 ± 126	295 ± 139	295 ± 200

^aAmine refers to mPEG-Amine, SMB refers to mPEG-SMB, NPM refers to NHS-PEG-MAL

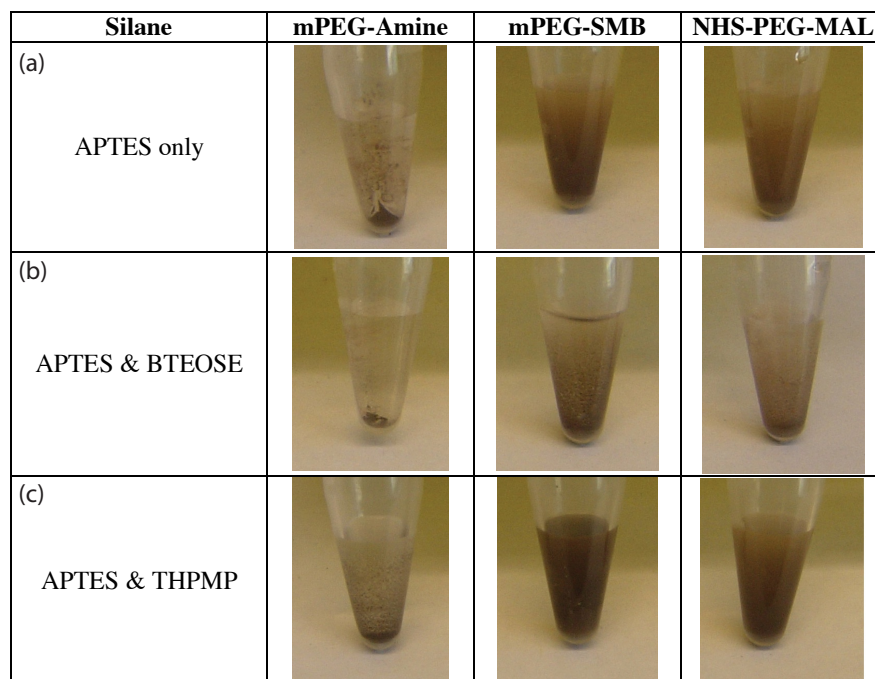


FIG. S2: **Stability of pegylated silicon nanoparticles.** Stability of pegylated particles after two days in PBS and gentle flicking, post amination with (a) APTES, (b) APTES and BTEOSE, and (c) APTES and THPMP.

Particle stability was also assessed visually, as shown in Fig. S2. These particles were pegylated in methanol, washed, and re-suspended in PBS. The particles treated with mPEG-Amine could not be re-suspended, as they had formed a large aggregate at the bottom of the tube. After two days in solution, some of the particles pegylated with mPEG-SMB and NHS-PEG-MAL had settled but immediately re-dispersed after gentle flicking.

* These authors contributed equally to this work

† To whom correspondence should be addressed (marcus@harvard.edu)

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